

Quantumness of spin-1 states

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(Dated: October 28, 2015)

We investigate quantumness of spin-1 states, defined as the Hilbert-Schmidt distance to the convex hull of spin coherent states. We derive its analytic expression in the case of pure states as a function of the smallest eigenvalue of the Bloch matrix and give explicitly the closest classical state for an arbitrary pure state. Numerical evidence is provided that the exact formula for pure states provides an upper bound on the quantumness of mixed states. Due to the connection between quantumness and entanglement we obtain new insights into the geometry of symmetric entangled states.

PACS numbers: 03.65.Aa, 03.65.Ca, 03.67.-a

I. INTRODUCTION

The quantum world is the realm of the most counter-intuitive phenomena, from the tunnel effect to the more recent quantum teleportation. There are, however, instances of quantum states which behave in an almost classical way. The best-known example of such a behavior is that of coherent states. With the rise of quantum information technology the need to identify genuine quantum states, where truly quantum phenomena could occur, has become important. Several notions of “quantumness” exist, emphasizing different physical consequences of quantum behaviour. One of the oldest ones goes back to quantum optics, where coherent states of light are considered the most classical pure states possible. These are states with minimal quantum uncertainty in the quadratures, i.e. localized as much as possible in phase space, and this property is preserved under the free time evolution of the electro-magnetic field [1]. The purely classical procedure of randomly choosing such states adds classical noise but no quantum noise. The resulting mixed states, whose Glauber representation is a convex sum of coherent state density matrices, form a convex set of states with positive P -function, and there is widespread agreement that such states are to be considered the most classical states [2, 3].

This definition was extended to finite-dimensional systems in [4], where spin-coherent states ($SU(2)$ coherent states) play the role of the pure states with minimal quantum fluctuations of the angular-momentum operators [5]. This property is conserved under unitary operations representing rotations. A mixed state can be considered classical if it can be written as a statistical mixture of spin coherent states, meaning that a representation with a positive P -function exists. The set of “classical spin states” can thus be defined as the convex hull of spin coherent states [4, 6]. Any state outside this set may be considered truly quantum. To measure the departure from the classical behaviour it is convenient to define “quantumness” as the Hilbert-Schmidt distance from the state to the set of classical states [6, 7]. Other quantifiers of quantumness are based on different sets of “classical states”, e.g. states with positive Wigner

function [8], and use various measures of distance, such as the trace distance [9] or the Bures distance [10].

Alternative measures of quantumness are based on entanglement [11–13]. Even though formal analogies of entanglement can be found also in classical physics, and have attracted attention recently in optics [14], entanglement is a signature of a quantum behaviour. Entangled quantum states can lead to stronger-than-classical correlations between subsystems. A number of entanglement measures have been proposed in order to quantify entanglement. A way of defining such a measure is to consider the distance between a state and the convex set of separable states. While this distance was shown to yield a good measure of entanglement when it is taken as the relative entropy or the Bures distance [15, 16], it is currently still unclear whether the Hilbert-Schmidt distance yields a good measure of entanglement [17], as it is not contractive [18]. However, this measure is mathematically convenient as a Euclidean distance on Hilbert space, and has nice physical properties. For instance the Hilbert-Schmidt distance is equal to the maximum amount by which a certain type of a generalized Bell inequality is violated [19]. Furthermore, we show here that the Hilbert-Schmidt distance gives new insight into the geometry of entangled states.

In the present paper, we investigate the problem of finding the distance from a state to the set of classical states, as well as the classical state closest to a given state. The closely related problem of finding the *separable* state closest to a given state has already been investigated in the literature. For instance, if one restricts the set of separable states to pure states then it was shown in [20] that the closest separable pure state in terms of Bures distance to a pure symmetric state is always symmetric. This result also holds for the Hilbert-Schmidt distance as both distances are simply related to the overlap of the two states in this pure state case. In [21], the problem of the Hilbert-Schmidt distance from a bipartite two qubit state to the closest (possibly mixed) separable state was investigated. Specializing the results of [21] to symmetric

states, one can observe that the separable state closest to a symmetric state (pure or not) is in general mixed and not necessarily symmetric.

Here we solve the problem of finding the classical state closest to a general spin-1 state, in terms of the Hilbert-Schmidt distance. We find an analytical solution for pure states. Our findings generalize a result obtained in [7] for the most quantum spin-1 pure state. As we will see, this also solves the problem of finding the symmetric separable state closest to a pure symmetric bipartite state of two qubits.

The paper is organized as follows. In Section II we introduce the Bloch matrix representation that we will use throughout the paper. Section III solves the problem of finding the classical state closest to any given pure spin-1 state, while Section IV tackles the problem for mixed states. Section V makes the connection with entanglement and entanglement measures.

II. DEFINITIONS

A. Tensor representation

A way of representing spin- j states which is particularly convenient when dealing with spin coherent states is the tensor representation proposed in [22]. It is a generalization of the well-known Bloch picture for spin- $\frac{1}{2}$ states. In the case $j = \frac{1}{2}$, any state ρ can be expanded as

$$\rho = \frac{1}{2} \sum_{\mu=0}^3 X_{\mu} S_{\mu}, \quad (1)$$

with S_0 the 2×2 identity matrix, and $S_i = \sigma_i$, $1 \leq i \leq 3$, the three Pauli matrices. In this basis, the coordinates of ρ are $X_0 = 1$ and $X_i = \text{tr}(\rho S_i)$, so that $\mathbf{X} = (X_1, X_2, X_3)$ forms the usual Bloch vector.

For higher spin, it is possible to associate to any spin- j state ρ a tensor with $2j$ indices [22]. For spin-1 this tensor reduces to a matrix that can be defined as

$$X_{\mu\nu} = \text{tr}(\rho S_{\mu\nu}), \quad 0 \leq \mu, \nu \leq 3, \quad (2)$$

with $S_{00} = \mathbb{1}$, the 3×3 identity matrix, $S_{a0} = S_{0a} = J_a$, and $S_{ab} = J_a J_b + J_b J_a - \delta_{ab} \mathbb{1}$, where J_a is the usual spin-1 angular momentum operator, $1 \leq a, b \leq 3$ (here we take $\hbar = 1$). The matrices $S_{\mu\nu}$ are such that ρ can be expanded as

$$\rho = \frac{1}{4} \sum_{\mu, \nu=0}^3 X_{\mu\nu} S_{\mu\nu}. \quad (3)$$

The 4×4 matrix X is real and symmetric with trace two. As in the spin- $\frac{1}{2}$ case, where the Bloch vector transforms as a three-dimensional vector under rotations of the coordinate frame, for spin-1, X transforms under a 3D rotation according to $X' = R X R^\dagger$, with R_{ab} , $1 \leq a, b \leq 3$,

the 3×3 rotation matrix, and $R_{0\mu} = R_{\mu 0} = \delta_{\mu 0}$, $0 \leq \mu \leq 3$. We will thus call X the Bloch matrix.

This representation is particularly well-suited to our problem, since, as we will see, coherent states take a very simple form in this framework.

B. Quantumness

The set \mathcal{C} of classical spin states is defined [4] as the ensemble of all density matrices which can be expressed as a mixture of spin coherent states with positive weights, i.e. states ρ_c for which there exist weights $w_i \geq 0$ and coherent states $|\alpha_i\rangle$ such that

$$\rho_c = \sum_i w_i |\alpha_i\rangle \langle \alpha_i|, \quad (4)$$

with $0 \leq w_i \leq 1$, and $\sum_i w_i = 1$. Here we use the following definition of spin coherent states $|\alpha\rangle = |\theta, \phi\rangle$, with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$ the usual spherical angles,

$$|\alpha\rangle = \sum_{m=-j}^j \sqrt{\binom{2j}{j+m}} \left(\cos \frac{\theta}{2}\right)^{j+m} \left(\sin \frac{\theta}{2} e^{-i\phi}\right)^{j-m} |j, m\rangle, \quad (5)$$

where $|j, m\rangle$ is the usual spin basis, here with $j = 1$ and $m = -1, 0, 1$.

The Bloch matrix of a coherent state takes the simple form $X_{\mu\nu} = n_{\mu} n_{\nu}$, $0 \leq \mu, \nu \leq 3$, with $n_0 = 1$ and $\mathbf{n} = (n_1, n_2, n_3) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. The decomposition (4) can be reexpressed in terms of the Bloch matrix W of ρ_c as

$$W_{\mu\nu} = \text{tr}(\rho_c S_{\mu\nu}) = \sum_i w_i n_{\mu}^{(i)} n_{\nu}^{(i)}, \quad (6)$$

with $\mathbf{n}^{(i)} = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$ the Bloch vectors corresponding to coherent states $|\alpha_i\rangle$ and $n_0^{(i)} = 1$.

Quantumness of an arbitrary state ρ can be defined [7] as the (Hilbert-Schmidt) distance to the convex set \mathcal{C} . Namely, the quantumness $Q(\rho)$ is given by

$$Q(\rho) = \min_{\rho_c \in \mathcal{C}} \|\rho - \rho_c\|, \quad (7)$$

where $\|A\| = \sqrt{\text{tr}(A^\dagger A)}$ is the Hilbert-Schmidt norm. Using Eq. (3), one can show that the quantumness can be re-expressed in terms of Bloch matrices as

$$Q(\rho) = \frac{1}{2} \min_{W \text{ classical}} \|X - W\|, \quad (8)$$

where X is the Bloch matrix of ρ and W is given by (6).

In [4], a necessary and sufficient criterion for classicality in the spin-1 case was obtained. A spin-1 state is classical if and only if the 3×3 matrix Z defined (using the present notation) by $Z_{ab} = X_{ab} - X_{a0} X_{b0}$, with $1 \leq a, b \leq 3$, is positive semi-definite. Remarkably, the

matrix Z is nothing but the Schur complement of the 1×1 upper left block of matrix X (note that $X_{00} = 1$). Therefore positive semi-definiteness of Z is equivalent to positive semi-definiteness of X . In other words, a spin-1 state is classical if and only if its matrix X is positive semi-definite. Equivalently, a spin-1 state is quantum if and only if the smallest eigenvalue of its matrix X is negative.

The Bloch matrix thus provides a simple classicality criterion. In the case of pure states, it also allows one to obtain an exact expression for the quantumness (7). This is the goal of the next section.

III. PURE STATES

Starting from a one-dimensional parametrization of pure states, we now prove a lower bound to the minimization problem (7) and then show that this lower bound can be reached by a classical state. This gives an analytic expression for Q for all pure states.

A. Parametrization

The Majorana representation [23, 24] allows one to uniquely map any pure spin- j state to $2j$ points on the Bloch sphere. If the pure state undergoes a unitary transformation $e^{i\varphi \mathbf{J} \cdot \mathbf{n}}$ that represents a rotation of angle φ about vector \mathbf{n} then the Majorana points are rotated rigidly by that rotation. Under such a transformation, coherent states are rotated into coherent states, so that from its definition it is clear that quantumness is invariant under rotation of the coordinate system. Moreover, since X transforms under rotations as explained in Section II A, its eigenvalues are unchanged under such rotations.

The Majorana representation of a spin-1 pure state $|\psi\rangle$ just consists of two points on the unit sphere. These points correspond, via the stereographic projection $z = \cot \frac{\theta}{2} e^{i\phi}$, to the roots of the Majorana polynomial $P(z) = d_1 - \sqrt{2}d_0z + d_{-1}z^2$, with $d_m, -1 \leq m \leq 1$, the coefficients of the state $|\psi\rangle$ in the $|j, m\rangle$ basis. The sphere (or the spin-1 state) can always be rotated in such a way that these two Majorana points are brought to a canonical position where they have spherical coordinates $(\theta, \phi) = (\gamma, 0)$ and $(\pi - \gamma, 0)$ without changing quantumness. States with Majorana points at positions $(\gamma, 0)$ and $(\pi - \gamma, 0)$ are given (up to normalisation \mathcal{N}) by

$$|\psi_\gamma\rangle = \mathcal{N} \left(|1, -1\rangle + \frac{\sqrt{2}}{\sin \gamma} |1, 0\rangle + |1, 1\rangle \right), \quad (9)$$

with $\gamma \in [0, \pi/2]$. We will use this expression as a canonical form for spin-1 pure states. The corresponding Bloch

matrix X is given by

$$X = \begin{pmatrix} 1 & \sqrt{1-\lambda^2} & 0 & 0 \\ \sqrt{1-\lambda^2} & 1 & 0 & 0 \\ 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix}, \quad (10)$$

with

$$\lambda = \frac{\sin^2 \gamma - 1}{\sin^2 \gamma + 1}. \quad (11)$$

The eigenvalues of X are $\pm\lambda$ and $1 \pm \sqrt{1-\lambda^2}$. When γ varies in $[0, \pi/2]$, λ varies in $[-1, 0]$, so that the smallest eigenvalue (and the only negative one) is λ . We will use λ as the parameter for spin-1 pure states.

According to the criterion of Section II B, a state ρ is classical if and only if X is positive semi-definite, that is, if and only if $\lambda \geq 0$. For pure states, since $\lambda \in [-1, 0]$ this implies that $\lambda = 0$. The Bloch matrix (10) then corresponds to the Bloch matrix of a coherent state with vector $\mathbf{n} = (1, 0, 0)$. Another way of seeing this is to note that $\lambda = 0$ is equivalent to $\gamma = \pi/2$, which corresponds to both Majorana points coinciding, i.e. a coherent state. We recover the known fact that the only classical pure states are coherent states.

B. Lower bound for the full range

We now show that for an arbitrary pure state $|\psi\rangle$ whose Bloch matrix X has smallest eigenvalue λ , quantumness is such that

$$Q(|\psi\rangle) \geq -\sqrt{\frac{3}{8}}\lambda. \quad (12)$$

Without loss of generality, the quantumness of $|\psi\rangle$ can be calculated by first transforming it to the canonical form (9). Then we write the quantumness (8) as

$$Q(|\psi\rangle) = \frac{1}{2} \min_{W \text{ classical}} \sqrt{\sum_{\mu\nu=0}^3 (X_{\mu\nu} - W_{\mu\nu})^2}, \quad (13)$$

with W of the form (6) and X given by (10). In order to obtain (12) it is sufficient to show that $\sum_{\mu\nu} (X_{\mu\nu} - W_{\mu\nu})^2 \geq \frac{3}{2}\lambda^2$ for all classical states W . This is possible by proving:

$$(X_{\mu\nu} - W_{\mu\nu})^2 \geq 0, \quad (14)$$

$$(X_{33} - W_{33})^2 - \lambda^2 \geq 0, \quad (15)$$

$$(X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 - \frac{\lambda^2}{2} \geq 0. \quad (16)$$

The first claim is true for all μ, ν , since the entries of X and W are real numbers. Using (10), condition (15) can be rewritten as

$$(|\lambda| + W_{33})^2 - \lambda^2 \geq 0, \quad (17)$$

which obviously holds since $W_{33} = \sum_i w_i \cos^2 \theta_i \geq 0$. In order to prove (16), we define $a = (W_{11} + W_{22})$ and $b = (W_{11} - W_{22})$. Then one can show the identity

$$(X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 - \frac{\lambda^2}{2} = \frac{1}{2} [(1-a)^2 - 2\lambda(1-a) + (\lambda+1-b)^2]. \quad (18)$$

Noting that $a = \sum_i w_i \sin^2 \theta_i \in [0, 1]$ and $\lambda \leq 0$, it immediately follows that this quantity is non-negative, which completes the proof of (12).

C. Exact value of $Q(|\psi\rangle)$ for $\lambda \in [-1, -\frac{1}{2}]$

It turns out that in the parameter range $\lambda \in [-1, -\frac{1}{2}]$ there is a classical state at precisely the distance given by the lower bound (12). We consider the family of states of the form

$$\begin{aligned} \rho_c(w, \beta) = & (1-2w)|\frac{\pi}{2}, 0\rangle\langle\frac{\pi}{2}, 0| \\ & + w|\frac{\pi}{2}, \beta\rangle\langle\frac{\pi}{2}, \beta| + w|\frac{\pi}{2}, -\beta\rangle\langle\frac{\pi}{2}, -\beta|, \end{aligned} \quad (19)$$

which are classical by construction for $w \in [0, 1/2]$, since they are a mixture of coherent states $|\theta, \phi\rangle$. By calculating the unconstrained minimum

$$\min_{w, \beta} |||\psi\rangle\langle\psi| - \rho_c(w, \beta)||, \quad (20)$$

the optimal choices for the parameters w and β are found to be

$$w = \frac{(4\lambda + 2)(1 - \sqrt{1 - \lambda^2}) - \lambda^2}{17\lambda + 8} \quad (21)$$

and

$$\beta = \arccos\left(\frac{-\sqrt{1 - \lambda^2} - 2\lambda - 1}{2\lambda}\right). \quad (22)$$

The condition $w \in [0, 1/2]$ translates to $\lambda \leq -1/2$. For these values the Bloch matrix of the state (19) reduces to

$$W = \begin{pmatrix} 1 & \sqrt{1 - \lambda^2} & 0 & 0 \\ \sqrt{1 - \lambda^2} & 1 + \frac{\lambda}{2} & 0 & 0 \\ 0 & 0 & -\frac{\lambda}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (23)$$

Note that since the set of classical states is closed and convex [4], there is a unique closest state to any given state for the (Euclidean) Hilbert-Schmidt distance. Since the distance from the state W to the state X (10) is exactly the value of the lower bound, it shows that W represents the closest classical state (ccs) for $|\psi\rangle$ in the range of $\lambda \in [-1, -\frac{1}{2}]$.

If $\lambda > -\frac{1}{2}$ the state corresponding to (23) does not represent a quantum state any more, since the corresponding density matrix is no longer positive. Actually, in the next section we find a tighter lower bound for $\lambda \in]-\frac{1}{2}, 0]$, which in particular implies that the distance between a quantum state and the set \mathcal{C} is larger than $\sqrt{3/8}|\lambda|$ for $\lambda \in]-\frac{1}{2}, 0]$. This proves that no classical state exists in this range $\lambda \in]-\frac{1}{2}, 0]$ that saturates the bound (12).

D. Tighter bound in the range $\lambda \in]-\frac{1}{2}, 0]$

In this section we show that for $\lambda \in]-\frac{1}{2}, 0]$ one has

$$Q(|\psi\rangle) \geq \frac{1}{2}\sqrt{\lambda^2 + \ell(\lambda)}, \quad (24)$$

where $\ell(\lambda)$ is given by

$$\begin{aligned} \ell(\lambda) = & \frac{1}{216} \left[3h^5 \sqrt{\frac{1 - \lambda}{(\lambda + 1)^3}} - \frac{6h^2(\lambda^2 - 52\lambda + 55)}{\lambda + 1} \right. \\ & \left. + h^4 - 216h\sqrt{1 - \lambda^2} + 72(11 - 4\lambda^2 + 4\lambda) \right] \end{aligned} \quad (25)$$

with

$$h = 6^{1/3} \left[9\sqrt{1 - \lambda^2} + \sqrt{3(\lambda + 1)(25 - 31\lambda - 2\lambda^2)} \right]^{1/3}. \quad (26)$$

The bound (24) is tighter than the one obtained in Section III B, as can be shown by proving that over the range $\lambda \in]-\frac{1}{2}, 0]$ one has

$$\frac{\sqrt{\lambda^2 + \ell(\lambda)}}{2} > -\sqrt{\frac{3}{8}}\lambda \quad (27)$$

(see end of the Appendix).

In order to prove the lower bound (24) it is sufficient to show that $\sum_{\mu\nu} (X_{\mu\nu} - W_{\mu\nu})^2 \geq \lambda^2 + \ell(\lambda)$ for all classical states. This is possible by proving:

$$(X_{\mu\nu} - W_{\mu\nu})^2 \geq 0, \quad (28)$$

$$(X_{33} - W_{33})^2 - \lambda^2 \geq 0, \quad (29)$$

$$(X_{11} - W_{11})^2 + (X_{22} - W_{22})^2 + 2(X_{01} - W_{01})^2 \geq \ell(\lambda). \quad (30)$$

Conditions (28) and (29) were already proven in the previous section, so we only have to show (30). This can be done by analytically calculating the minimal value of the left-hand side of (30) under the restrictions on the values of $W_{\mu\nu}$ implied by Eq. (6). For readability, we rewrite the left-hand side of (30), using the form (10) for a general pure state Bloch matrix X and Eq. (6) for a general classical state W as

$$F(u, v, g) := (1 - u)^2 + (\lambda + v)^2 + 2(\sqrt{1 - \lambda^2} - g)^2 \quad (31)$$

with $u = \sum_i w_i \sin^2 \theta_i \cos^2 \phi_i$, $v = \sum_i w_i \sin^2 \theta_i \sin^2 \phi_i$, and $g = \sum_i w_i \sin \theta_i \cos \phi_i$. These new variables are such that

$$\begin{aligned} u + v &\leq 1 \\ u, v &\geq 0 \\ -\sqrt{u} &\leq g \leq \sqrt{u}. \end{aligned} \quad (32)$$

The last condition is derived from Jensen's inequality $(\sum_i w_i a_i)^2 \leq \sum_i w_i a_i^2$ with $a_i = \sin \theta_i \cos \phi_i$. The minimum of $F(u, v, g)$ under the constraints (32) can be calculated analytically, and, as shown in the Appendix, it is equal to $\ell(\lambda)$ given in (25). This proves Eq. (30), and thereby the tighter lower bound (24) for the range $\lambda \in]-\frac{1}{2}, 0]$.

E. Exact value of $Q(|\psi\rangle)$ for $\lambda \in]-\frac{1}{2}, 0]$

The tighter lower bound (24) can be reached in the range of $\lambda \in]-\frac{1}{2}, 0]$, since there are classical states at this distance. Using a similar approach as in Section III C, we consider a family of classical states of the form

$$\rho_c(\beta) = \frac{1}{2} \left(\left| \frac{\pi}{2}, \beta \right\rangle \left\langle \frac{\pi}{2}, \beta \right| + \left| \frac{\pi}{2}, -\beta \right\rangle \left\langle \frac{\pi}{2}, -\beta \right| \right), \quad (33)$$

which are a mixture of just two coherent states $|\theta, \phi\rangle$ with equal weights $\frac{1}{2}$. Let a pure state $|\psi\rangle$ have a Bloch matrix with smallest eigenvalue λ . The state $\rho_c(\beta)$ closest to the canonical form (9) of $|\psi\rangle$ is determined by the condition

$$\frac{\partial}{\partial \beta} |||\psi\rangle\langle\psi| - \rho_c(\beta)|| = 0, \quad (34)$$

which has the solution $\beta = \arccos d$, with d defined as the real root of the polynomial

$$P(y) = \sqrt{1 - \lambda^2} + y(1 + \lambda) - 2y^3, \quad (35)$$

where $\lambda \in]-\frac{1}{2}, 0]$, corresponding to $d \in]\frac{\sqrt{3}}{2}, 1]$. Using this value of β gives the Bloch matrix of ρ_c as

$$W = \begin{pmatrix} 1 & d & 0 & 0 \\ d & d^2 & 0 & 0 \\ 0 & 0 & 1 - d^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (36)$$

The state represented by (36) is then exactly at the distance to the pure state (10) given by the tighter lower bound (24). Therefore we have proven that the classical state closest to (10) is (36) for the parameter range $\lambda \in]-\frac{1}{2}, 0]$.

F. Summary of results for pure states

To conclude, let an arbitrary pure spin-1 state $|\psi\rangle$ be given by its Bloch matrix (2). If the smallest eigenvalue

of X is denoted by λ , then the quantumness of $|\psi\rangle$ is equal to the quantumness of a state with Bloch matrix (10), and takes the form

$$Q(|\psi\rangle) = f(\lambda), \quad (37)$$

with

$$f(\lambda) := \begin{cases} -\sqrt{\frac{3}{8}}\lambda & \text{for } \lambda \leq -\frac{1}{2}, \\ \frac{1}{2}\sqrt{\lambda^2 + \ell(\lambda)} & \text{for } \lambda > -\frac{1}{2}, \end{cases} \quad (38)$$

and $\ell(\lambda)$ given by Eq. (25). The function $f(\lambda)$ is shown in Fig. 1. It is continuous at $\lambda = -\frac{1}{2}$. At this plot scale, $f(\lambda)$ is almost indistinguishable from a linear function.

The maximal difference between $f(\lambda)$ and $-\sqrt{\frac{3}{8}}\lambda$ is less than 0.0016 over the interval $[-1, 0]$.

The classical states closest to a pure state $|\psi\rangle$ take a different expression in the two regions $\lambda < -\frac{1}{2}$ and $\lambda > -\frac{1}{2}$, respectively given by (23) and (36). In contrast to the case of the queen of quantum for $j = 1$, corresponding to $\lambda = -1$ [7], these closest classical states (ccs) are not simply a mixture of the pure state $|\psi\rangle$ itself and the maximally mixed state, i.e. for $\lambda \neq -1$

$$\text{ccs} \neq a|\psi\rangle\langle\psi| + (1-a)\frac{\mathbb{1}}{3}, \quad 0 \leq a \leq 1. \quad (39)$$

IV. MIXED STATES

1. Mixed state quantumness

For pure states we obtained the analytical expression (37) for quantumness as a function of a single parameter, namely the smallest eigenvalue λ of the Bloch matrix of the state. In this Section we investigate the dependence of $Q(\rho)$ as a function of λ for mixed states. For a given state ρ the quantumness can be obtained numerically by determining the closest classical state of ρ . To find this state we randomly generate a large sample of coherent states $\{|\theta_i, \phi_i\rangle\}$ (5), and then optimize the weights w_i of this decomposition

$$\rho_c = \sum_i w_i |\theta_i, \phi_i\rangle\langle\theta_i, \phi_i|, \quad (40)$$

so that the distance from ρ to ρ_c is minimal. As the function Q^2 defined in (7) corresponds to the minimization of a function which is quadratic in the w_i , this optimization can be done by quadratic programming. The result of the optimization yields an approximation of the quantumness: In general it is overestimated by this approach, as coherent states appearing in the decompositions of the closest classical state may not be included in our random sample. However, this overestimated value is very close to the true value. Indeed, for pure states, where the analytic expression (37) is available, the error incurred by the numerical approach is typically of the order of

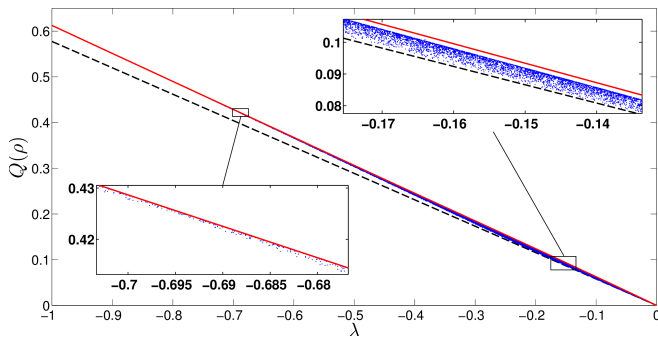


FIG. 1. (Color online) Quantumness of randomly generated mixed states, as a function of the smallest eigenvalue of their Bloch matrix. There are 50000 points, each one corresponding to a random state. Red line corresponds to the pure states analytic result $f(\lambda)$ given by Eq. (38). Dashed line indicates the lower bound (45). Function $f(\lambda)$ appears to be an upper bound on the quantumness of mixed states (see inset).

$\sim 10^{-6}$ for the numerical data in this paper. This can be also checked on mixed states, for instance by increasing the number of coherent states involved in the sum (40), or by changing the choice of coherent states in the random list: Our results show that the results obtained are quite independent on increasing the number of coherent states over which we optimize (further detail on our optimization procedure will be given elsewhere [25]).

In Fig. 1 we plot the quantumness of mixed states as a function of the smallest eigenvalue of their Bloch matrix. Since, from the classicality criterion $X \geq 0$, non-classical states are such that $\lambda \in [-1, 0[$, we restrict our plot to this interval (note that for classical states λ takes positive values, while the quantumness is zero by definition). The mixed states were randomly generated from the Hilbert-Schmidt ensemble of matrices $\rho = AA^\dagger / \text{tr}(AA^\dagger)$, with A a complex matrix with independent Gaussian entries (see [26] for detail). All points lie very close to the pure state result. This signifies that quantumness of a mixed state appears to largely depend on a single parameter, which is the smallest eigenvalue of its Bloch matrix, although mixed states cannot be reduced to a one-parameter family (as is the case for pure states, up to rotations).

2. Upper bound for quantumness of mixed states

The function $f(\lambda)$ appears to be an upper bound for the quantumness of mixed states, namely

$$Q(\rho) \leq f(\lambda), \quad (41)$$

with λ the smallest eigenvalue of the Bloch matrix of ρ . This can be seen in the inset of Fig. 1. More precisely, Fig. 2 displays the difference between the quantumness and $f(\lambda)$ as a function of the smallest eigenvalue of the Bloch matrix. In fact, we were not able to find a single state which violates the bound. It may happen that, for

states very close to pure states, the numerical overestimation of quantumness due to our optimization procedure leads to a result larger than $f(\lambda)$; however by increasing the accuracy of our estimation (that is, taking more coherent states in the sum (40)), we were always able to get this estimate back below the threshold $f(\lambda)$. Numerical evidence thus suggests that this upper bound is valid for all mixed states.

The almost empty region in the upper right corner of Fig. 2 (visible also just below the upper bound in the upper inset of Fig. 1) corresponds to the region between $f(\lambda)$ and the straight line $-\sqrt{3/8}\lambda$ in the interval $[-\frac{1}{2}, 0]$. This apparent emptiness just comes from our numerical sampling: indeed, this region can be filled e.g. by points corresponding to mixed states of the form

$$\rho = a|\psi\rangle\langle\psi| + (1-a)\text{ccs}(|\psi\rangle) \quad (42)$$

with $0 \leq a \leq 1$ and $|\psi\rangle$ a pure state with closest classical state $\text{ccs}(|\psi\rangle)$ and $\lambda \in [-\frac{1}{2}, 0]$.

In the special case where a mixed state ρ can be written as a convex combination of a pure state and its closest classical state ccs , as in (42), Eq. (41) can be proven. This can be shown by the fact that $\|\rho - \text{ccs}(|\psi\rangle)\| = aQ(\psi)$, so that $Q(\rho) \leq af(\lambda_\psi)$, with λ_ψ the smallest eigenvalue of the Bloch matrix of $|\psi\rangle$. By using the explicit form of f given by (38), one can show that $af(\lambda_\psi) \leq f(a\lambda_\psi)$, for $0 \leq a \leq 1$ (this is true for $-1 \leq \lambda \leq -1/2$ because of the inequality (27), and for $-1/2 \leq \lambda \leq 0$ by concavity of f over this interval). From the forms (10) and (23),(36) of the Bloch matrices, one can show that for states (42) the smallest eigenvalue of the Bloch matrix of ρ is given by $\lambda = a\lambda_\psi$, hence (41). This proves the upper bound for the family of states (42). However a proof for arbitrary mixed states is still missing.

3. Lower bound for quantumness of mixed states

The quantumness of mixed states can be bound from below by minimizing over a larger set than in Eq. (8) (see [21] for a similar approach). Let X be the Bloch matrix of some state ρ and λ be the smallest eigenvalue of X . A lower bound can be obtained as

$$\frac{1}{2} \min_{W \text{ classical}} \|X - W\| \geq \frac{1}{2} \min_{\tilde{W}, \tilde{X}} \|\tilde{X} - \tilde{W}\|, \quad (43)$$

where \tilde{W} runs over all positive semi-definite matrices with $\text{tr} \tilde{W} = 2$, and \tilde{X} runs over all real symmetric matrices with one eigenvalue equal to λ and $\text{tr} \tilde{X} = 2$. Furthermore, we can write \tilde{X} in its diagonal form $\tilde{X} = \text{diag}(x_1, x_2, x_3, \lambda)$ with x_i arbitrary real numbers since the norm and the set over which \tilde{W} runs in the rhs of Eq. (43) are invariant under orthogonal transformations.

Because \tilde{X} is diagonal the optimal \tilde{W} will also be in diagonal form. Since \tilde{W} is positive, let $\tilde{W} = \text{diag}(w_1^2, w_2^2, w_3^2, w_4^2)$, with real w_i such that $\sum_{i=1}^4 w_i^2 = 2$.

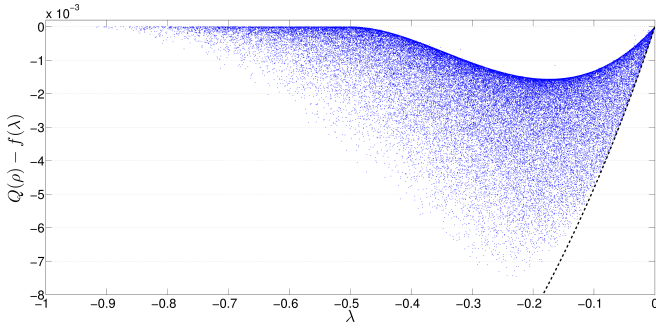


FIG. 2. Difference between the quantumness and the hypothetical upper bound $f(\lambda)$ as function of the smallest eigenvalue of the Bloch matrix (same data as in Fig. 1). The difference between the upper bound and the quantumness is of the order of 10^{-3} . The numerical error is of order 10^{-6} , and our numerical procedure can only overestimate quantumness so that the points could only be lower than they appear here by that amount. The dashed line corresponds to the lower bound (45).

The right hand side of (43) can then be rewritten as

$$\frac{1}{2} \min_{\substack{x_i, w_i \in \mathbb{R} \\ \sum_{i=1}^3 x_i = 2 - \lambda \\ \sum_{i=1}^4 w_i^2 = 2}} \left[(\lambda - w_4^2)^2 + \sum_{i=1}^3 (x_i - w_i^2)^2 \right]^{1/2}. \quad (44)$$

This is a simple problem of minimization under constraints, which can be solved by introducing appropriate Lagrange multipliers. When λ is negative (non-classical states), the critical points of the Lagrange function are found to be such that either $w_i = 0$ for $1 \leq i \leq 3$, or $w_4 = 0$. The latter case yields the smallest value for the quantumness, which is equal to $-\frac{\lambda}{\sqrt{3}}$. So the quantumness of any mixed state ρ with smallest eigenvalue λ of its Bloch matrix is bound by

$$Q(\rho) \geq -\frac{\lambda}{\sqrt{3}}. \quad (45)$$

This lower bound corresponds to the dashed line in Figs. 1 and 2. For small enough quantumness, the two bounds provided in this section are close to tight in the sense that the quantumness of random mixed states extends almost over the whole range between them.

V. CONNECTION WITH ENTANGLEMENT

We now establish a connection between quantumness and entanglement, and relate the smallest eigenvalue of the Bloch matrix to known entanglement measures such as the negativity and the concurrence.

A. Entanglement

A bipartite pure state $|\psi\rangle$ is called separable if it can be written as a direct product of pure states of its subsystems

$$|\psi\rangle = |\psi^{(1)}\rangle \otimes |\psi^{(2)}\rangle. \quad (46)$$

This definition can be extended to mixed states: a bipartite mixed state is called separable if it can be written as a convex sum of tensor products of quantum states of the subsystems,

$$\rho = \sum_i w_i \rho_i^{(1)} \otimes \rho_i^{(2)}, \quad (47)$$

where the w_i are classical probabilities with $w_i \geq 0$ and $\sum_i w_i = 1$. If a state cannot be written in this form then it is called entangled [27].

For two spin- $\frac{1}{2}$ states, entanglement can be detected by use of the partial transpose [28]. The necessary and sufficient 'positive partial transpose' (PPT) criterion [29] states that a state is separable if and only if ρ^{PT} is positive semi-definite, where $^{\text{PT}}$ denotes the partial transpose operation.

In order to quantify entanglement, commonly used measures are the negativity and the concurrence. The negativity is given as

$$\mathcal{N}(\rho) = \sum_i \frac{|\mu_i| - \mu_i}{2}, \quad (48)$$

where μ_i are the eigenvalues of ρ^{PT} . The concept of negativity is also connected to the concept of robustness of entanglement [30].

The concurrence C was developed as an analytic solution of the entanglement of formation for two spins- $\frac{1}{2}$ [31]. For a two spin- $\frac{1}{2}$ state ρ it is given as

$$C(\rho) = \max\{0, \tau_1 - \tau_2 - \tau_3 - \tau_4\}, \quad (49)$$

where τ_i are the square roots of the eigenvalues of the matrix

$$\rho(\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y) \quad (50)$$

in decreasing order, and $*$ denotes the complex conjugation. In Section V C we will relate these entanglement measures with quantumness. We first discuss the analogy between classicality and separability.

B. Classicality and separability

Classicality is a property defined for a spin- j state. It is interesting to look at a spin- j state as the projection of a tensor product of $2j$ spin- $\frac{1}{2}$ states onto the subspace symmetric under permutation of the particles. Any basis vector $|j, m\rangle$ then appears as a symmetrized $2j$ -fold tensor product.

The symmetric subspace of two spin- $\frac{1}{2}$ states is spanned by the Dicke states

$$|D_0\rangle = |\uparrow\uparrow\rangle, \quad |D_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad |D_2\rangle = |\downarrow\downarrow\rangle. \quad (51)$$

The basis vector $|1, m\rangle$ corresponds to $|D_{1-m}\rangle$ for $-1 \leq m \leq 1$. Identifying (in $|j, m\rangle$ notation) $|\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle = |\downarrow\rangle$, the tensor product of spin- $\frac{1}{2}$ coherent states (5) is

$$\left(\cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{-i\phi}|\downarrow\rangle\right)^{\otimes 2} = \cos^2\frac{\theta}{2}|D_0\rangle + \sqrt{2}\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{-i\phi}|D_1\rangle + \sin^2\frac{\theta}{2}e^{-2i\phi}|D_2\rangle \quad (52)$$

which, from the correspondence $|1, m\rangle = |D_{1-m}\rangle$, is equivalent to

$$|\alpha\rangle^{j=\frac{1}{2}} \otimes |\alpha\rangle^{j=\frac{1}{2}} = |\alpha\rangle^{j=1} \quad (53)$$

where $|\alpha\rangle^j$ is a spin- j coherent state given by (5). Thus the spin-1 coherent states are separable in the tensor product space. Therefore, all classical states of the form (4), as mixtures of coherent states, can be identified with separable states.

Conversely, a two qubit symmetric separable state $\rho_s = \sum_i w_i \rho_i^{(1)} \otimes \rho_i^{(2)}$ with $w_i > 0$ can be identified with a classical spin-1 state. Indeed, if ρ_s is symmetric then

$$\langle D^- | \rho_s | D^- \rangle = 0, \quad (54)$$

with $|D^- \rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. This is equivalent to

$$\sum_i w_i \langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = 0. \quad (55)$$

Since all summands are non-negative (by positivity of density matrices) it follows that

$$\langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = 0 \quad \forall i. \quad (56)$$

If the qubit states $\rho^{(1,2)}$ are written with the Bloch vectors $\mathbf{X}^{(1,2)}$ according to Eq. (1), direct calculations give

$$\langle D^- | \rho_i^{(1)} \otimes \rho_i^{(2)} | D^- \rangle = \frac{1}{4}(1 - \mathbf{X}^{(1)} \cdot \mathbf{X}^{(2)}). \quad (57)$$

Because the Bloch vectors are such that $\|\mathbf{X}^{(1,2)}\| \leq 1$, Eq. (57) implies that $\mathbf{X}^{(1)} = \mathbf{X}^{(2)}$ and $\|\mathbf{X}^{(1,2)}\| = 1$. Thus $\rho_i^{(1)} = \rho_i^{(2)}$, which corresponds to the same pure qubit state $|\alpha_i\rangle\langle\alpha_i|^{j=1/2}$. Therefore one can write

$$\rho_s = \sum_i w_i |\alpha_i\rangle\langle\alpha_i|^{j=1/2} \otimes |\alpha_i\rangle\langle\alpha_i|^{j=1/2}. \quad (58)$$

With (53) it follows that ρ_s can be identified with

$$\sum_i w_i |\alpha_i\rangle\langle\alpha_i|^{j=1}, \quad (59)$$

which represents a classical state (4). Thus, the set of classical spin-1 states can be identified with the set of separable symmetric states of two qubits.

This equivalence can also be shown indirectly using the PPT criterion. Indeed, there is a remarkable connection between the partial transpose of a state ρ and the Bloch matrix X of ρ . Namely, one can easily check that

$$\rho^{\text{PT}} = \frac{1}{2} R X R^\dagger \quad (60)$$

with the unitary matrix

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -i & 0 \\ 0 & 1 & i & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}. \quad (61)$$

Therefore the Bloch matrix is nothing but the partial transpose of ρ expressed in a different basis. As shown in section IIB, a necessary and sufficient condition for classicality is that X be positive semi-definite. As the eigenvalues are unchanged by the change of basis (60) (but for a factor $\frac{1}{2}$), this condition is equivalent to the positive semi-definiteness of ρ^{PT} , which in turn is equivalent to separability. In other words, this proves that a spin-1 state is entangled (when seen as a bipartite system) if and only if its quantumness is non-zero.

Any separable state can be written in the form (47), with possibly $\rho_i^{(1)} \neq \rho_i^{(2)}$. If that state lies in the subspace spanned by (51), then necessarily, from the considerations above, $\rho_i^{(1)} = \rho_i^{(2)}$, so that ρ can be cast in the form

$$\rho = \sum_i w_i \rho_i \otimes \rho_i, \quad (62)$$

with ρ_i spin- $\frac{1}{2}$ coherent states, that is, a form where the particle-exchange invariance appears also on the level of the density matrix.

C. Quantumness and entanglement

In Section III and IV we related quantumness of a state ρ to the smallest eigenvalue of its Bloch matrix (2). If this smallest eigenvalue is denoted by λ , then from the correspondence (60), the smallest eigenvalue of ρ^{PT} is equal to $\lambda/2$. In the case of a bipartition of two spin- $\frac{1}{2}$ states, ρ^{PT} has at most one negative eigenvalue [32], so that negativity (48) reduces to $\mathcal{N}(\rho) = -\lambda/2$. In the case of pure states, the concurrence defined in (49) reduces to

$$C(|\psi\rangle\langle\psi|) = -\lambda. \quad (63)$$

Of course, as is expected for pure states, the negativity and the concurrence are simply related by $C(|\psi\rangle\langle\psi|) = 2\mathcal{N}(|\psi\rangle\langle\psi|)$ [32].

The function $f(\lambda)$ defined in (38) thus allows us to express quantumness as function of negativity for pure spin-1 states. For mixed spin-1 states Eq. (41) becomes

$$d_{HS}(\rho, \mathcal{C}) \leq f(-2\mathcal{N}(\rho)), \quad (64)$$

and as we showed equality holds for pure states. Furthermore, it gives an insight into the geometry of entangled states as it allows one to connect negativity to a geometric property, namely the Hilbert-Schmidt distance d_{HS} from an entangled state to the set \mathcal{C} of symmetric separable states. In general, since the closest separable state found in [21] is non-symmetric, the corresponding minimal Hilbert-Schmidt distance obtained in [21] is smaller than the one we get as we consider the distance to symmetric separable states only.

VI. CONCLUSION

In this paper we investigated the quantumness of spin-1 states, defined as Hilbert-Schmidt distance to the convex set of classical spin-1 states. We found the analytical solution for the quantumness $Q(|\psi\rangle)$ of arbitrary pure states. It can be expressed as a function of the smallest eigenvalue of the Bloch matrix associated with $|\psi\rangle$. For mixed states, the same function appears to give an upper bound for $Q(\rho)$ according to extensive numerical investigations. We established the connection of $Q(\rho)$ with entanglement measures.

The closest classical state also provides a classicality witness, in the spirit of [33]. Our derivations provide another example of the usefulness of the tensor representation of spin states [22].

Acknowledgments: We thank the Deutsch-Französische Hochschule (Université franco-allemande) for support, grant number CT-45-14-II/2015.

APPENDIX: ANALYTIC CALCULATION OF THE MINIMA

Here we will calculate the minimal value of F defined in (31) under the constraints (32). If $\lambda = 0$, the minimum of F is zero. We exclude this case in the following for convenience and restrict ourselves to the interval $\lambda \in] -1/2, 0[$. We will use the fact that the minimal value of a function, restricted to a certain parameter range, has its minimal value either on a critical point or at the border of the parameter range. This will give a list of candidates for the global minimum. The smallest value in this list is then the global minimum.

To calculate the minimal value, we distinguish two cases, $u \geq 1 - \lambda^2$ and $u < 1 - \lambda^2$. In each case we can simplify the problem by setting the variable g to its optimal value. In the first case $D := F(g = \sqrt{1 - \lambda^2})$ so that the third term vanishes, and in the second case

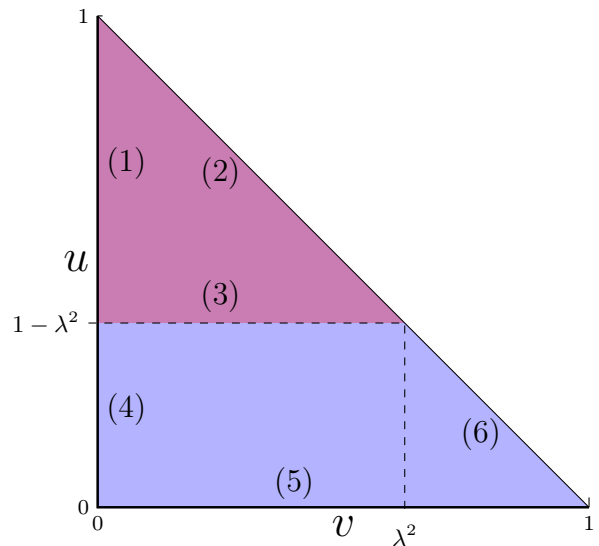


FIG. 3. Visualisation of the allowed parameter range of the variables u and v . The upper area corresponds to $u \geq 1 - \lambda^2$, while the lower corresponds to $u \leq 1 - \lambda^2$. We call the function $F(u, v, g)$ restricted to the upper (lower) area D (E).

$E := F(g = \sqrt{u})$, which makes the last term as small as possible.

In both cases the new functions

$$D = (1 - u)^2 + (\lambda + v)^2, \quad (65)$$

$$E = (1 - u)^2 + (\lambda + v)^2 + 2(\sqrt{1 - \lambda^2} - \sqrt{u})^2 \quad (66)$$

do not have critical points in the allowed parameter range of u and v (32), since $\nabla_{u,v} D = 0$ is only solved by $(u, v) = (1, -\lambda)$, which is outside the parameter range for $\lambda < 0$, and $\nabla_{u,v} E = 0$ is only solved by $(u, v) = (\sqrt[3]{1 - \lambda^2}, -\lambda)$, which is also outside the parameter range for $\lambda < 0$, since it contradicts the condition $u + v \leq 1$. Therefore both functions have to have their minimal value on the borders of the parameter range depicted in Fig. 3. The function D restricted to the line (1) in Fig. 3 will be referred to as D^1 , analogues D^2 , D^3 . These three functions do not have a critical point on the interior of their respective parameter ranges, so the minimal value must be in all three cases on one of the two vertices. Consider the candidates for the minimal value for the function D , as

$$\left. \begin{array}{l} D^1(u = 1) \\ D^2(v = 0) \end{array} \right\} = \lambda^2 \quad (67)$$

$$\left. \begin{array}{l} D^1(u = 1 - \lambda^2) \\ D^3(v = 0) \end{array} \right\} = \lambda^4 + \lambda^2 \quad (68)$$

$$\left. \begin{array}{l} D^2(v = \lambda^2) \\ D^3(v = \lambda^2) \end{array} \right\} = \lambda^2 (2\lambda^2 + 2\lambda + 1). \quad (69)$$

Comparing these values the minimal value of D is found to be $\lambda^2 (2\lambda^2 + 2\lambda + 1)$.

The minimum of the function E will be calculated analogously. The function on the line (3) in Fig. 3 will be referred to as E^3 , similar E^4 on line (4), and so forth. The function E^3 is the same as D^3 so its minimal value is also $\lambda^2(2\lambda^2 + 2\lambda + 1)$.

The function $E^4(u) = (1-u)^2 + \lambda^2 + 2(\sqrt{1-\lambda^2} - \sqrt{u})^2$ has a critical value at $u = \sqrt[3]{1-\lambda^2}$, which is larger than $1-\lambda^2$, and therefore outside the allowed range of the lower area in Fig. 3. So the minimal value is reached at the second of the two edges

$$E^4(u=0) = 3 - \lambda^2, \quad (70)$$

$$E^4(u=1-\lambda^2) = \lambda^4 + \lambda^2. \quad (71)$$

The function $E^5(v) = 1 + (v+\lambda)^2 + 2(1-\lambda^2)$ has a critical value in the allowed parameter range, at $v = -\lambda$, corresponding to a minimum

$$E^5(v=-\lambda) = 3 - 2\lambda^2. \quad (72)$$

The function $E^6(u) = (1-u)^2 + (\lambda+1-u)^2 + 2(\sqrt{1-\lambda^2} - \sqrt{u})^2$ has a critical value in the allowed parameter range of $u \in [0, 1-\lambda^2]$. The condition $\partial_u E^6 = 0$ gives

$$1 + \lambda + \frac{\sqrt{1-\lambda^2}}{\sqrt{u}} - 2u = 0, \quad (73)$$

with the substitution $u = y^2$ the optimal value of u is

given through the real root d of

$$\sqrt{1-\lambda^2} + y(1+\lambda) - 2y^3 = 0, \quad (74)$$

which is the same polynomial as in (35). The second derivative

$$\frac{\partial^2 E^6}{\partial u^2} = \frac{\sqrt{1-\lambda^2}}{u^{3/2}} + 4 \quad (75)$$

is positive over the whole parameter range, so the critical point is a minimum, with value

$$\ell(\lambda) = E^6(u=d^2). \quad (76)$$

With this list of local minima, for all possible cases, the global minimum of (31) is found to be (76), which yields (25).

Proving Eq. (27) is equivalent to showing that $\ell(\lambda) \geq \frac{\lambda^2}{2}$. We have $E^6 \geq \frac{\lambda^2}{2}$, since

$$E^6 - \frac{\lambda^2}{2} = 2\left(\sqrt{u} - \sqrt{1-\lambda^2}\right)^2 + \frac{1}{2}[\lambda + 2(1-u)]^2, \quad (77)$$

which, as the sum of squares, is always non-negative. Therefore the minimum of E^6 is also larger or equal to $\frac{\lambda^2}{2}$. As an immediate consequence, inequality (27) holds.

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